

# Parity violating effects in an exotic perturbation of the rigid rotator

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**Abstract** The perturbation of the free rigid rotator by the trigonometric Scarf potential is shown to conserve its energy excitation patterns and change only the wave functions towards spherical harmonics rescaled by a function of an unspecified parity, or mixtures of such rescaled harmonics of equal magnetic quantum numbers and different angular momenta. In effect, no parity can be assigned to the states of the rotational bands emerging in this exotic way, and the electric dipole operator is allowed to acquire non-vanishing expectation values.

**Keywords:** rigid rotator, trigonometric Scarf potential, degeneracy conservation, parity violation, non-vanishing electric dipole moment

## 1 Introduction

The energy spectra of molecules consisting of two atoms are as a rule well understood in terms of equidistant vibrational excitations characterized by wavelengths in the millimetric infrared range, on top of which one observes rotational bands of energies growing as  $J(J+1)$ , with  $J$  non-negative integer, which disintegrate by emitting nanometric microwave radiations (so called rovibron model [1]). For a fixed vibrational mode, the microwave radiation is entirely attributed to the proportionality of the molecular Hamiltonian to the squared angular momentum operator,  $\mathbf{J}^2$ ,

$$\mathcal{H}_{rot}(\theta, \varphi) = \frac{\hbar^2}{2\mu R_e^2} \mathbf{J}^2(\theta, \varphi), \quad \mathbf{J}^2(\theta, \varphi) = -\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} - \frac{\frac{\partial^2}{\partial \varphi^2}}{\sin^2 \theta}, \quad (1)$$

where  $\mu$  stands for the reduced mass of the two molecules, and  $R_e$  denotes the equilibrium bound length. The description of the rotational modes amounts to the diagonalizing of  $\mathcal{H}_{rot}(\theta, \varphi)$  in the basis of the functions,  $\Phi(\theta, \varphi)$  of the polar,  $\theta$ , and azimuthal,  $\varphi$ , angles,

$$\mathcal{H}_{rot}(\theta, \varphi) \Phi(\theta, \varphi) = E \Phi(\theta, \varphi). \quad (2)$$

Interpreting  $\mu R_e^2$  as the moment of inertia,  $\mathcal{I}$ , about the center of mass, the equation (2) is cast in the standard form of the linear rigid rotor, termed to here as rigid rotator, according to,

$$\mathcal{B} \mathbf{J}^2(\theta, \varphi) Y_J^M(\theta, \varphi) = E_J Y_J^M(\theta, \varphi), \quad E_J = \mathcal{B} J(J+1), \quad \mathcal{B} = \frac{\hbar^2}{2\mathcal{I}}, \quad (3)$$

with  $\mathcal{B}$  being the rotational constant. The solutions to the latter equation are the well known three-dimensional spherical harmonics,  $Y_J^M(\theta, \varphi)$ , i.e.  $\Phi(\theta, \varphi) = Y_J^M(\theta, \varphi)$ , defined as,

$$Y_J^M(\theta, \varphi) = e^{iM\varphi} P_J^M(\cos \theta), \quad J = 0, 1, 2, \dots \quad (4)$$

Here,  $P_J^M(\cos \theta)$  are the associated Legendre functions [2], known to become the Legendre polynomials,  $P_J(\cos \theta)$ , for  $M = 0$ . It is of common use to cast the rotational spectrum in (3) in terms of frequencies,  $\nu(J)$ , as

$$\nu(J) = \frac{1}{h} E_{rot} = \frac{1}{h} (E_J - E_{(J-1)}) = 2 \frac{\mathcal{B}}{h} J, \quad (5)$$

and define spectral lines separated by the constant gap of  $2\mathcal{B}/h$ . The above considerations refer to the idealized case of a pure rotator, the reality being that the equidistant line spacings are altered by

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centrifugal distortions and other secondary effects, left aside in what follows. The rotational spectra are remarkable through the fact that the energy,  $E_J$ , equivalently, the frequency,  $\nu(J)$ , in (5), depends on  $J$  alone meaning that the multiplicity of states in a level is  $(2J + 1)$ -fold. Also the shapes of the disintegration (“radiation”) patterns, more precisely, the angular probability density distributions, given by the spherical polar plots of the squared  $Y_J^M(\theta, \varphi)$  functions, are energy degenerate. The plot in fig. 1 illustrates the degeneracy of the probability density distributions responsible for the disintegration of the states  $|J = 1, M = 0, \pm 1\rangle$  to the ground state.

Our principal goal is to answer the question whether the shapes of the probability density distributions are uniquely determined by the spectral frequencies, which parallels the celebrated question asked by Mark Kac in 1966, on whether the sound frequencies of a drum specify its form in an unique way [3]. Our case is that similarly to Kac’s question, also the answer to the one posed here by us turns out to be negative.

Our point is that the perturbation of  $\mathcal{H}_{rot}(\theta, \varphi)$  by a properly designed potential can retain the spectral frequencies and alter the wave functions. In this fashion, two sets of identical isospectral frequency patterns will correspond to two sets of probability density distributions of non-equivalent shapes. Stated differently, according to our findings,  $(2J + 1)$ -fold degeneracies do not necessarily imply equality of the Hamiltonian neither to the one of the canonical rigid rotator, nor to a similarity transformation of it. To be specific, below we show that the energies in the spectrum of the rigid rotator, perturbed by the trigonometric Scarf potential, remain identical to those within the spectrum of the free rotator, though the wave functions of the former are of unspecified parities and quite distinct from those of the latter, which are the spherical harmonics of well defined parities. The consequence will be rotational levels of non-vanishing electric dipole moments. The paper is structured as follows. In the next section we place the goal of our investigation within the context of spectral geometry and isospectral potentials. In section 3 we introduce the perturbation of the rigid rotator by the trigonometric Scarf potential and present its spectrum and wave functions. In section 4 we analyze the wave functions emerging after the perturbation and show they have lost their spatial parities, thus allowing for non-vanishing electric dipole expectation values. The paper closes with brief conclusions.

## 2 Isospectral potentials from the perspective of spectral geometry

Spectral geometry studies the relation between spectral properties of elliptic differential or pseudo-differential operators and the associated Riemannian manifolds, among them curved surfaces. A Riemannian manifold,  $(M, g)$ , is characterized by its metric  $g$  with covariant components,  $g_{\alpha\beta}$ , and its Laplacian which is a second order differential operator acting on symmetric traceless tensors of second ranks, viewed as infinitesimal metric transformations. The general definition of a Laplacian in the spirit of Lichnerowicz reads,  $\Delta_g = -\text{div}(\nabla) = -\nabla^\alpha \nabla_\alpha = -g^{\beta\gamma} \nabla_\beta \nabla_\gamma$ , with the minus sign ensuring a spectrum bounded from below.

A further key characteristic of a curved surface, in the following restricted to a compact Riemannian space, is the eigenvalue problem of the Laplace operator,  $\Delta_g$  on this metric,

$$\Delta_g f_k = \lambda_k f_k, \quad i = 0, 1, 2, \dots \quad (6)$$

with  $f_k$  being the corresponding eigenfunctions. The discrete number sequence,  $(0 =) \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \dots \rightarrow \infty$  is referred to as the spectrum of  $\Delta_g$ , or, of  $M$ . The vibrations of a thin membrane (a drum) are fixed by the eigenfunctions of the relevant Laplacian with Dirichlet boundary conditions and the square roots,  $\sqrt{\lambda_i}$ , of the eigenvalues are proportional to the sound frequencies. The fundamental questions asked by mathematicians in spectral geometries (see [4] for a pedagogical text) concern the properties of the spectrum given the geometry (the metric) and vice versa, whether the geometry (the metric) can be restored given the spectrum. While the first question is straightforwardly answered by solving the eigenvalue problem of the Laplacian, the answer to the inverse spectrum problem is far from being obvious. The issue is that the information provided by the spectrum alone is insufficient to allow one to uniquely recover the metric of the surface. Mark Kac’s question mentioned in the introduction on whether one can hear the shape of a drum [3] expresses precisely this very non-uniqueness of the solutions of the inverse spectral problem. Indeed, several drums of strictly equal spectra and non-equivalent shapes have been constructed beginning with work by Gordon and Wilson in 1984 [5]. The applications of spectral geometry to physics are highly interesting and allow one to handle the so called isospectral potential problems [6]. The latter refer to two flat space Schrödinger equations with distinct potentials,  $V_1$  and  $V_2$ ,

$$H^{(1)} \psi_i^{(1)} = \left( -\frac{\hbar^2}{2M} \nabla^2 + V_1 \right) \psi_i^{(1)} = E_i^{(1)} \psi_i^{(1)},$$

$$\begin{aligned} H^{(2)}\psi_i^{(2)} &= \left(-\frac{\hbar^2}{2M}\nabla^2 + V_2\right)\psi_i^{(2)} = E_i^{(2)}\psi_i^{(2)}, \\ E_i^{(1)} &= E_i^{(2)} \equiv E_i, \end{aligned} \quad (7)$$

which nonetheless describe exactly same spectra. Here,  $M$  denotes the mass of the particle under consideration. Several such potential pairs are known in quantum mechanics, the Morse and the hyperbolic Scarf potentials being one of them (see [7] for details). In one of the possibilities, though not necessarily, two isospectral potentials can be related by a so called isospectral transformation which is no more than a similarity transformation of any one of the Hamiltonians, say  $H^{(1)}$ , by some properly selected invertible smooth function,  $\mathbf{F}$ , according to

$$H^{(2)}\psi_i^{(2)} = [\mathbf{F}H^{(1)}\mathbf{F}^{-1}] [\mathbf{F}\psi_i^{(1)}] = E_i [\mathbf{F}\psi_i^{(1)}], \quad (8)$$

meaning

$$V_2 = [\mathbf{F}H^{(1)}\mathbf{F}^{-1}] + \frac{\hbar^2}{2M}\nabla^2, \quad \psi_i^{(2)} = \mathbf{F}\psi_i^{(1)}. \quad (9)$$

In general, potentials generated in this manner are complicated and contain gradient terms. The link of the Schrödinger equation to geometry (so called “geometrization” of Schrödinger’s equation [8]) is established on the basis of the observation that the equations in (7) equivalently rewrite to eigenvalue problems of Laplacians in the so-called Maupertuis-Jacobi metrics, here denoted by  $g_{ij}^{(MJ)}(V_k)$  and defined as,

$$g_{ij}^{(MJ)}(V_k) = \Omega^2 \delta_{ij}, \quad \Omega^2 = 2M(E_i - V_k), \quad k = 1, 2, \quad (10)$$

as

$$\begin{aligned} \left(\hbar^2 \widetilde{\nabla}^2_{g^{(MJ)}(V_k)} + 1\right) \psi_i^{(1)} &= 0 \\ \widetilde{\nabla}^2_{g^{(MJ)}(V_k)} &= \Omega^{-2} \nabla^2. \end{aligned} \quad (11)$$

Here,  $\Omega^2$  is the so called “conformal” factor. Correspondingly, the metrics  $g_{ij}^{(MJ)}(V_k)$  are referred to as conformal, while  $\widetilde{\nabla}^2_{g^{(MJ)}(V_k)}$  are the conformal Laplacians on the surfaces with the Maupertuis -Jacobi metrics,  $g^{(MJ)}(V_k)$  (with  $k = 1, 2$ ). It should be obvious that the equations in (11) refer to isospectral problems on surfaces of distinct metrics and can be treated with the methods of spectral geometry, as indicated in the opening of this section.

Back to the inverse spectral problem, in order to restore its uniqueness, new information needs to be invoked. As such, mathematicians consider the numbers of nodes and the nodal lines of the eigenfunctions [9]. Within the context of spectral geometry the goal of the present study can be cast in the following way:

We draw attention to the fact that the angular potentials

$$V_1(\theta) = \frac{M^2 - \frac{1}{4}}{\cos^2 \theta}, \quad V_2(\theta) = \frac{M^2 - \frac{1}{4} + b^2}{\cos^2 \theta} - \frac{2bM \tan \theta}{\cos \theta} - \frac{1}{4}, \quad (12)$$

are isospectral.

However, rather than explicitly constructing the respective Maupertuis-Jacobi metrics, we here, being focused on physical applications in general, and on molecular physics in particular, prefer to visualize the difference of the aforementioned metrics indirectly. In first place the distinction is made through the evidently different shapes of the  $V_1(\theta)$  and  $V_2(\theta)$  probability density distributions corresponding to equal quantum numbers and same energy, and in second place through the unspecified parities of the  $V_2(\theta)$  eigenfunctions, in contrast to the well defined parities of the  $V_1(\theta)$  eigenfunctions. These are all physical entities of high spectroscopic relevance and are of major interest to experimental studies of the disintegration modes.

Another interesting question regarding isospectral potentials concerns their symmetry properties. As we shall see in the following, the  $V_1(\theta)$  potential is rotationally invariant because in properly chosen coordinates, it can be viewed as part of the Laplace operator on the two-dimensional spherical surface,

$S^2$ . The symmetry properties of the second potential are not instantly obvious and need to be elaborated separately. For this purpose one first has to systematically search for a complete set of operators which commute with  $\widehat{\nabla}^2_{g^{(M,J)}(V_2)}$  and then investigate their commutators with the aim to possibly figure out a relevant Lie algebra. This question, in going far beyond the scope of our investigation, will be left aside for the time being, and will be attended properly in a future work. The next section is devoted to the presentation of our case.

### 3 Exotic degeneracy preserving perturbation of the rigid rotator

In the current section we choose to simplify notations for the sake of transparency of the formulas and work in dimensionless units, setting  $\mathcal{B} = 1$ . In eq. (2) the parametrization of the two dimensional sphere is such that the polar angle  $\theta$  has been read off from the positive  $z$  axis (the North pole). Instead, we here take the liberty (without any loss of generality) to read off this angle from the negative  $y$ -axis, meaning that instead of tracing meridians in the usual way along North-East-South-West-North direction, we trace them along West-North-East-South-West. The reason behind this re-parametrization of the sphere will be explained shortly below, after the equation (21). In so doing, the expression for  $\mathbf{J}^2$  and the spherical harmonics correspondingly changes to,

$$\mathbf{J}^2(\theta, \varphi) = -\frac{1}{\cos \theta} \frac{\partial}{\partial \theta} \cos \theta \frac{\partial}{\partial \theta} + \frac{J_z^2}{\cos^2 \theta} = -\frac{\partial^2}{\partial \theta^2} + 2 \tan \theta \frac{\partial}{\partial \theta} - \frac{M^2}{\cos^2 \theta}, \quad (13)$$

$$\mathbf{J}^2(\theta, \varphi) Y_J^M(\theta, \varphi) = J(J+1) Y_J^M(\theta, \varphi), \quad (14)$$

$$J_z(\varphi) = -i \frac{\partial}{\partial \varphi}, \quad Y_J^M(\theta, \varphi) = e^{iM\varphi} P_J^M(\sin \theta). \quad (15)$$

With that in mind, we now consider the perturbation of the rigid-rotator by the following potential,  $\mathcal{V}(\theta)$ ,

$$\begin{aligned} \mathbf{J}^2(\theta, \varphi) &\rightarrow H(\theta, \varphi) = \mathbf{J}^2(\theta, \varphi) + \mathcal{V}(\theta), \\ \mathcal{V}(\theta) &= \frac{b^2}{\cos^2 \theta} - \frac{2bM \tan \theta}{\cos \theta} - \frac{1}{4}. \end{aligned} \quad (16)$$

The eigenvalue problem of the perturbed Hamiltonian now takes the form,

$$H(\theta, \varphi) \Psi(\theta, \varphi) = \epsilon \Psi(\theta, \varphi), \quad \Psi(\theta, \varphi) = \phi(\theta) e^{iM\varphi}. \quad (17)$$

The second order operator (13) contains a first order derivative, which can be eliminated under the following variable change,

$$U(\theta) = \sqrt{\cos \theta} \phi(\theta). \quad (18)$$

In effect, (16) acquires the shape of the following one-dimensional (1D) Schrödinger equation in the  $\theta$  variable,

$$\mathcal{H}(\theta) U(\theta) = \epsilon U(\theta), \quad \mathcal{H}(\theta) = \left[ -\frac{d^2}{d\theta^2} + V_{ScI}(\theta) \right], \quad (19)$$

with the Schrödinger perturbation potential, here denoted by  $V_{ScI}(\theta)$ , being given as,

$$\begin{aligned} V_{ScI}(\theta) &= \frac{b^2 + a(a+1)}{\cos^2 \theta} - \frac{b(2a+1) \tan \theta}{\cos \theta} - \frac{1}{4}, \\ a &= |M| - \frac{1}{2}. \end{aligned} \quad (20)$$

The squared magnetic quantum number,  $M^2$ , in the operator on the sphere in (13), gets replaced in the one-dimensional Schrödinger operator by,

$$M^2 \rightarrow M^2 - \frac{1}{4} = a(a+1) = \left( |M| - \frac{1}{2} \right) \left( |M| + \frac{1}{2} \right), \quad (21)$$

and acquires meaning of an ordinary potential parameter.

According to the nomenclature in [7], the singular interaction,  $V_{ScI}(\theta)$  in (20) is known under the name of the trigonometric Scarf potential, abbreviated, “Scaf I”. This nomenclature, though strictly speaking at variance with Scarf’s original work [10], where a  $\csc^2$  singular potential has been considered, pays tribute

to the  $\text{sech}^2$  interaction, commonly named in the literature as hyperbolic Scarf potential, to which it relates by a complexification of the argument directly and without the need of introducing an additional shift by  $\pi/2$ . Instead, the  $\text{csc}^2$  potential, according to same nomenclature, is referred to as Pöschl-Teller potential with emphasis on [11] where a combined  $\text{csc}^2 + \text{sec}^2$  interaction has been introduced for the first time. Admittedly, other nomenclatures exist [12] according to which  $\text{csc}^2$  is referred to as trigonometric Scarf potential. As it will become clear in due course shortly below, after eq. (25), the nomenclature does not affect the results.

The singular  $\mathcal{H}(\theta)$  eigenvalue problem is known to be exactly solvable and has been well elaborated in the literature. The general method consists in finding a suited point-canonical transformation that reduces the Schrödinger equation to the hypergeometric differential equation, known to have three regular singular points [13], namely at  $x = 0$ ,  $x = 1$ , and at infinity. At regular points, the solutions can be expanded in Frobenius series which in the case under consideration happen to terminate and give rise to Jacobi polynomials. This method has been pioneered by Stevenson as early as 1941 in [14]. Alternatively, such equations can also be handled by the so called factorization method underlying modern super-symmetric quantum mechanics (see [7] for details), or by employing the recently elaborated Nikiforov-Uvarov method [15].

The solutions to (19) are given, among others, in [12]. Upon equipping the wave functions with quantum numbers according to,

$$U(\theta) \rightarrow U_t^{|M|}(\theta), \quad \epsilon \rightarrow \epsilon_t, \quad (22)$$

they are expressed as,

$$U_t^{|M|}(\theta) = \mathbf{W}(\theta) \cos^{|M|+\frac{1}{2}} \theta P_n^{|M|-b, |M|+b}(\sin \theta),$$

$$\mathbf{W}(\theta) = \left( \frac{1 + \sin \theta}{1 - \sin \theta} \right)^{\frac{b}{2}}, \quad \psi_t^M(\theta, \varphi) = U_t^{|M|}(\theta) e^{iM\varphi}, \quad (23)$$

$$\epsilon_t = t(t+1), \quad t = |M| + n, \quad |M| \in [0, t], \quad t = 0, 1, 2, \dots, \quad (24)$$

and with  $n$  standing for the degree of the Jacobi polynomial,  $P_n^{\alpha, \beta}(\sin \theta)$  [16]. Setting  $b = 0$  recovers (modulo the  $\sqrt{\cos \theta}$  factor in (18)) the solution of the free rigid rotator by equivalently re-expressing the spherical harmonics in terms of the Jacobi polynomials according to,

$$\frac{U_t^{|M|}(\theta)|_{b=0}}{\sqrt{\cos \theta}} = P_t^M(\sin \theta) = \cos^{|M|} \theta P_n^{|M|, |M|}(\sin \theta), \quad n = t - |M|. \quad (25)$$

The  $b = 0$  case corresponds to a Schrödinger equation with the  $\text{sec}^2 \theta$  potential  $V_1(\theta)$  in (12), while  $b \neq 0$  corresponds to (20), same as  $V_2(\theta)$  in (12). As long as the energy in (24) is  $b$  independent, the isospectrality of the potentials in (12) is revealed. Notice that because the polar angle in (13) has been read off from the negative  $y$ -axis instead as usual from the North Pole, the argument in the associated Legendre functions is  $\cos(\frac{\pi}{2} - \theta) = \sin \theta$  instead of the usual  $\cos \theta$ . In reality, we are dealing with Jacobi Polynomials of an argument  $x$  varying in the interval,  $-1 \leq x \leq 1$ , and both choices for  $x$ ,  $x = \sin \theta$ , with  $\theta \in [-\pi/2, +\pi/2]$ , or,  $x = -\cos \theta$  with  $\theta \in [0, \pi]$  are equally valid.

Accordingly, the parities of the wave functions, to be studied in the next section, are obtained from  $\theta \rightarrow -\theta$  and not from  $\theta \rightarrow \pi - \theta$ . Finally, the  $M$  values are restricted to natural numbers, satisfying the conditions,

$$|M| - b + 1 > 0, \quad |M| + b + 1 > 0, \quad (26)$$

as required to ensure the known orthogonality of the Jacobi polynomials on the interval  $-1 \leq \sin \theta \leq +1$ . As far as the  $|M|$  values are integer, this restriction implies  $|b| < 1$  for  $|M| = 0$ .

Comparison of (24) to (3)-(4), with both  $t$  and  $J$  taking same non-negative integer values, reveals the indistinguishability of the energy spectra of the free rigid rotator and the one perturbed by the trigonometric Scarf potential in the equations, (16)–(24). However the Scarf I wave functions in (23) are distinct from the spherical harmonics in (15), as it should be, given the non-commutativity of the squared angular momentum operator with this very potential, i.e.  $[\mathbf{J}^2(\theta, \varphi), V_{ScI}(\theta)] \neq 0$ . There is indeed no theorem which prevents two non-commuting operators of having equal eigenvalues. The operators non-commutativity only prohibits their simultaneous diagonalizing in same function basis.

Our findings on the exotic rotational bands parallel at the quantum level the non-equivalent isospectral classical drums [3] mentioned in the introduction.

The next section is devoted to the loss of parity of the wave functions of the perturbed rigid rotator under investigation.

#### 4 Parityless states and non-vanishing electric dipole moments

In the present section we study the relationship between the wave functions of the free and perturbed rotators. We begin with the simplest case of the ground state,  $t = 0$ , implying,  $n = M = 0$ . The corresponding wave function is read off from (23) as

$$\begin{aligned}\psi_0^0(\theta, \varphi) &= U_0^0(\theta)e^{i0\varphi}, \\ U_0^0(\theta) &= \sqrt{\cos\theta}\mathbf{W}(\theta) = \sqrt{\cos\theta}(1 + \sin\theta)^{\frac{1}{2}}(1 - \sin\theta)^{-\frac{1}{2}}.\end{aligned}\quad (27)$$

As a technical detail, we wish to notice that the ground state wave function,  $\psi_0^0(\theta, \varphi)$ , acts as the eigenfunction to an  $so(3)$  algebra Casimir invariant in a representation non-equivalent to the canonical one and defined by the following similarity transformation of the canonical squared angular momentum operator,  $\mathbf{J}^2$ , in (13):

$$\begin{aligned}\tilde{\mathbf{J}}^2(\theta, \varphi) &= \cos^{\frac{1}{2}}\theta\mathbf{W}(\theta)\mathbf{J}^2(\theta, \varphi)\mathbf{W}^{-1}(\theta)\cos^{-\frac{1}{2}}\theta, \\ \tilde{\mathbf{J}}^2(\theta, \varphi)\tilde{Y}_J^M(\theta, \varphi) &= J(J+1)\tilde{Y}_J^M(\theta, \varphi), \\ \tilde{Y}_J^M(\theta, \varphi) &= \sqrt{\cos\theta}\mathbf{W}(\theta)Y_J^M(\theta, \varphi).\end{aligned}\quad (28)$$

Indeed, the  $\tilde{\mathbf{J}}^2(\theta, \varphi)$  ground state,  $\tilde{Y}_0^0(\theta, \varphi)$ , satisfies

$$\tilde{\mathbf{J}}^2(\theta, \varphi)\tilde{Y}_0^0(\theta, \varphi) = 0, \quad (29)$$

whose obvious solution,

$$\tilde{Y}_0^0(\theta, \varphi) = \cos^{\frac{1}{2}}\theta\mathbf{W}(\theta)Y_0^0(\theta, \varphi), \quad Y_0^0(\theta, \varphi) = \sqrt{\frac{1}{4\pi}}, \quad (30)$$

coincides (modulo multiplicative constants) with  $\psi_0^0(\theta, \varphi)$  in (27). The  $\tilde{\mathbf{J}}^2$  eigenfunctions,  $\tilde{Y}_J^M(\theta, \varphi)$ , are obtained by rescaling the ordinary spherical harmonics,  $Y_J^M(\theta, \varphi)$ , by the transformation function,  $\sqrt{\cos\theta}\mathbf{W}(\theta)$ , and will be termed to as “rescaled harmonics”. However, due to the unspecified parity of the function,  $\mathbf{W}(\theta)$  in (28), which is transformed by reflection into its inverse,  $\mathbf{W}(-\theta) \rightarrow \mathbf{W}^{-1}(\theta)$ , rather than into itself up to a sign, all the rescaled harmonics are of unspecified parity. Related examples can be found in [17].

Our next example concerns the first excited state, corresponding to  $t = 1$ , and to the maximal allowed  $|M|$  value of  $|M| = 1$ , *i.e.*  $n = 0$ . One finds,

$$\begin{aligned}\psi_1^1(\theta, \varphi) &= U_1^1(\theta)e^{i\varphi} = \mathbf{W}(\theta)\cos^{\frac{3}{2}}\theta P_0^{-b,+b}(\sin\theta)e^{i\varphi} = \mathbf{W}(\theta)\cos^{\frac{3}{2}}\theta e^{i\varphi} \\ &= \sqrt{\cos\theta}\mathbf{W}(\theta)P_1^1(\sin\theta)e^{i\varphi} = \tilde{Y}_1^1(\theta, \varphi),\end{aligned}\quad (31)$$

and again an eigenfunction to the  $\tilde{\mathbf{J}}^2$   $so(3)$  Casimir invariant in (28),

$$\tilde{\mathbf{J}}^2(\theta, \varphi)\tilde{Y}_1^1(\theta, \varphi) = 2\tilde{Y}_1^1(\theta, \varphi). \quad (32)$$

In general, it can be shown that all wave functions of maximal  $|M| = t$  values (they include the ground state) behave as  $\tilde{\mathbf{J}}^2(\theta, \varphi)$  eigenfunctions and are characterized by a single angular momentum value, same that defines their energy. For all these states one is allowed to maintain the  $t$  label as a number conserved under transformations of the  $so(3)$  algebra in the representation defined in (29), despite the loss of the parity specification explained after the equation (30) above.

Next we consider the case of  $t = 2$  and  $|M| = 1$ , which corresponds to  $n = 1$ . We again express the relevant wave function  $\psi_2^1(\theta, \varphi)$  in terms of associated Legendre functions,  $P_J^{|M|}(\sin\theta)$ . In so doing, one finds

$$\begin{aligned}\psi_2^1(\theta, \varphi) &= \sqrt{\cos\theta}\mathbf{W}(\theta)\cos\theta P_1^{1-b,1+b}(\sin\theta)e^{i\varphi} \\ &= \sqrt{\cos\theta}\mathbf{W}(\theta)\cos\theta [-b + 2\sin\theta] e^{i\varphi}\end{aligned}$$

$$\begin{aligned}
&= \sqrt{\cos \theta} \mathbf{W}(\theta) [-b \cos \theta + 2 \cos \theta \sin \theta] e^{i\varphi} \\
&= \sqrt{\cos \theta} \mathbf{W}(\theta) \left[ -b P_1^1(\sin \theta) e^{i\varphi} + \frac{2}{3} P_2^1(\sin \theta) e^{i\varphi} \right] \\
&= \sqrt{\cos \theta} \mathbf{W}(\theta) \left[ -b Y_1^1(\theta, \varphi) + \frac{2}{3} Y_2^1(\theta, \varphi) \right] \\
&= -b \tilde{Y}_1^1(\theta, \varphi) + \frac{2}{3} \tilde{Y}_2^1(\theta, \varphi).
\end{aligned} \tag{33}$$

As long as the parity of the spherical harmonics is  $(-1)^J$ , the functions  $Y_1^1(\theta, \varphi)$ , and  $Y_2^1(\theta, \varphi)$  are of opposite parities, and  $\psi_2^1(\theta, \varphi)$  is built on top of a parity-mixed state. Moreover, the mixture of the rescaled harmonics in (33) no longer behaves as  $\tilde{\mathbf{J}}^2$  eigenstate, and the  $t = 2$  label in this case can not be interpreted as a quantum number conserved under transformations of the  $so(3)$  algebra in the representation of (29). Decompositions of the art presented in (33) can be performed for all the higher  $t$  values. They conserve the  $|M|$  label and mix (rescaled) spherical harmonics with  $J = |M|, \dots, t$ ,

$$\psi_t^M(\theta, \varphi) = \sum_{J=|M|}^{J=t} c_J \tilde{Y}_J^M(\theta, \varphi). \tag{34}$$

As a reminder, the  $\tilde{Y}_J^M(\theta, \varphi)$  functions, defined in (28), are always of unspecified parity. It is obvious that the electric dipole moment, whose selections rules are  $\Delta M = 0$ , and  $\Delta J = 1$ , will have a non-vanishing expectation value in the  $\psi_2^1(\theta, \varphi)$  state due to the allowed  $Y_2^1(\theta, \varphi) \rightarrow Y_1^1(\theta, \varphi)$  transition, on the one side, and more generally, due to the parityless nature of the  $\mathbf{W}(\theta)$  function, on the other side. We have checked that also the general integrals

$$d_e = \int [\psi_t^M(\theta, \varphi)]^* \sin \theta \psi_t^M(\theta, \varphi) \sin \theta d\theta d\varphi \neq 0, \tag{35}$$

are non-vanishing for  $b$  values satisfying the conditions in (26). We recall that the argument of the associated Legendre functions in these spherical harmonics is  $\sin \theta$ , versus  $\cos \theta$  in the standard ones. Finally a comment on the symmetry properties of the wave functions of the perturbed motion is in order. These can vary and are determined besides by the  $|M|$  value, as explained in the paragraph after eq. (32), also by the values of the  $b$  parameter. While for continuous  $b$  values the wave functions with  $|M| \neq t$  do not behave as  $\tilde{\mathbf{J}}^2$  eigenfunctions, for regular integer, or half-integer  $b$  values, call them  $b = M'$ , it can be shown that the Jacobi polynomials times  $\cos^{|M|} \theta$  would behave as Wigner's small  $d_{MM'}^t$  functions [18] and the rotational symmetry is respected. We here emphasize on continuous  $b$  values. Comparison of the ordinary spherical harmonics, the wave functions of the free rigid rotator, to the Schrödinger wave functions of the Scarf I- perturbed rotator, is presented in fig. 2.

## 5 Conclusions

In conclusion, pure rotational frequency patterns do not necessarily imply equality of the Hamiltonian to that of the canonical rigid rotator.

For discrete values of the potential parameter  $b$ , such patterns occur because the isospectral potentials in (12) are related through a similarity transformation of the type given in (8)-(9) with the place of  $\mathbf{F}$  being taken by the  $\cos^{\frac{1}{2}} \theta \mathbf{W}(\theta)$  factor in the wave function in (23). We discussed this issue after eq. (35). Stated differently, the Schrödinger Hamiltonian with the trigonometric Scarf potential for such parameter values is identical to the similarity transformed squared angular momentum operator,  $\tilde{\mathbf{J}}^2 = \cos^{\frac{1}{2}} \theta \mathbf{W}(\theta) \mathbf{J}^2 \cos^{-\frac{1}{2}} \theta \mathbf{W}^{-1}(\theta)$ , as explained in (28). Same happens when the magnetic quantum number  $|M|$  takes its maximal value. In all these cases the reason behind the rotational patterns of the perturbed motion is still the  $so(3)$  symmetry of the Hamiltonian, though in a representation distinct from the canonical one. However, for continuous  $b$  values the above considerations are no longer valid and the reason behind the rotational spectrum is not obvious. In order to get an insight into the symmetry properties of the perturbed Hamiltonian for this case one has to follow the standard procedure and find the complete set of operators with which it is commuting. In calculating the commutators of these operators, a clue on a possible Lie algebra might be obtained [19].

In all cases, the wave functions of the rigid rotator, perturbed by the trigonometric Scarf potential in (20), despite of the rotational multiplicity of the states in the levels, are in first place always of unspecified parities. In consequence, a sort of exotics is produced in so far as the states in the rotational bands acquire non-vanishing electric dipole moments. The symmetry behind the emerging exotic rotational spectrum

for continuous  $b$  values is not very clear so far. We conclude on the possibility for existence of exotic rotational bands containing parityless states in two-body systems of a possibly new class, be them di-atomic-, di-molecular, quarkish, etc. and whose states carry non-vanishing electric dipole expectation values.

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## References

- [1] C. D. Harris and M. D. Bertolucci, *Symmetry and Spectroscopy* (Oxford University Press, 1978).
- [2] G. B. Arfken and H.-J. Weber, *Mathematical methods for Physicists*, 5th ed. (Academic Press, 2001).
- [3] Mark Kac, *Can one hear the shape of a drum?*, Am. Math. Monthly, **73**, Issue 4, Part 2: Papers in Analysis (April, 1966) 1-23.
- [4] M. Vito Cruz, *The spectrum of the Laplacian in Riemannian geometry*, preprint 2003, <https://math.berkeley.edu/~alanw/240papers03/vitocruz.pdf>
- [5] C. S. Gordon and E. Wilson, *Isospectral deformations of compact manifolds*, J. Differential Geometry **19** (1984), 241-256.
- [6] Carolyn S. Gordon and Dorothee Schueth, *Isospectral potentials and conformally equivalent isospectral metrics on spheres, balls and Lie groups*, J. Geom. Analysis **13** (2) (2003) 279-3006. <http://www.math.hu-berlin.de/~schueth/confo.pdf>
- [7] A. Khare, *Supersymmetry in quantum mechanics*, + AIP Conference proceedings, **744** (2005) 133-165.
- [8] A. Karamtskou and H. Kleinert, *Geometrization of the Schrödinger equation: Application of the Maupertuis principle to quantum mechanics*, Int. J. Geom. Meth. Mod. Phys. **11** (2014) 14066-(1-15).
- [9] S. Gnutzman, U. Smilansky, and N. Sondergaard, *Resolving isospectral “drums” by counting nodal domains*, J. Phys. A: Math. Gen. **38** (2005) 8921-8933.
- [10] F. L. Scarf, *Discrete states for singular potential problems*, Phys. Rev. **109** (6) (1959) 2170-2176.
- [11] G. Pöschl and E. Teller, *“Bemerkungen zur Quantenmechanik des anharmonischen Oscillators”*, Z. Physik **83** (3-4) (1933) 143-151.
- [12] R. De, R. Dutt, and U. Sukhatme, *Mapping of shape invariant potentials under point canonical transformations*, J. Phys. A: Math. Gen. **25** (1992) L843-L850.
- [13] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis*, 3rd ed. (Cambridge University Press, 1920), Chpt. X, pp. 194–196.
- [14] A. F. Stevenson, *A note on the “Kepler problem” in a spherical space, and the factorization method of solving eigenvalue problems*, Phys. Rev. **59** (1941) 842-843.
- [15] C. Khari and A. Suprami, *Approximate solutions of Schrodinger equation for trigonometric Scarf Potential with the Poschl-Teller Non-central potential using NU method*, J. Appl. Phys. (IOSR-JAP), **2** (3) (2012) 13-33.
- [16] Phillipe Dennery and André Krzywicki, *Mathematics for Physicists* (Dover Publications, Mineola, New York, 1996).
- [17] Y. Alhassid, F. Gürsey, and F. Yachello, *Potential scattering, transfer matrix, and group theory*, Phys. Rev. Lett. **50** (1983) 873-876.
- [18] G. Lévai, F. Cannata, and A. Ventura,  *$\mathcal{PT}$ -symmetric potentials and the  $so(2,2)$  algebra*, J. Phys. A: Math. Gen. **35** (2002) 5041-5057.
- [19] A. Pallares-Rivera, F. de J. Rosales-Aldape, and M. Kirchbach, *Perturbing free motions on hyper-spheres without degeneracy lift*, J. Phys. A: Math. Theor. **47** (2014) 085303.



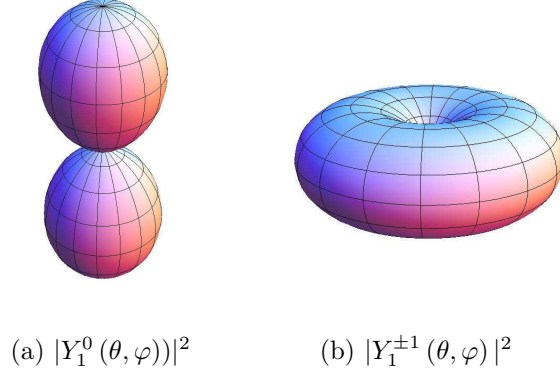


Figure 1: The three different shapes of the probability density distributions according to which one and the same energy, like  $E_{J=1} = 2\mathcal{B}$ , corresponding to the first excited level, is released in the  $|1M\rangle \rightarrow |00\rangle$  ground state transition, *i.e.* spherical polar plots of the  $|Y_1^0(\theta, \varphi)|^2$  and  $|Y_1^{\pm 1}(\theta, \varphi)|^2$  functions, defined in (4). The right figure counts twice because the radiation can go clockwise or, counter-clockwise.

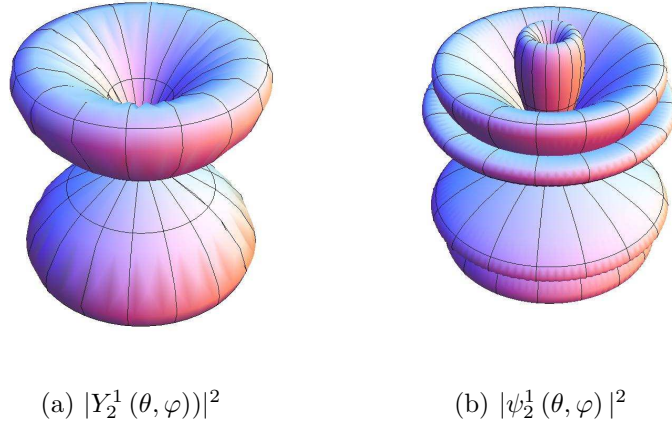


Figure 2: Illustration of how equal rotational energies (frequencies) can correspond to non-equivalent shapes of the probability density distributions. For the canonical rigid rotor, a probability density distribution of the release to the ground state of the energy,  $E_J = E_t = 6\mathcal{B}$ , of the second excited level, is given in fig. 2(a), while that corresponding to the perturbed rotator is displayed in fig. 2(b). The squared canonical rigid rotator wave function in fig. 2(a) is single  $J$ -valued, while the perturbed one in fig. 2(b) contains a  $\Delta J = 1$  mixture according to (33). The potential parameter  $b$  has been given the generic continuous value of,  $b = 0.45$ . The figure visualizes the statement that one can not "hear" the shape of the radiation patterns from the spectral frequencies.